The Uncertain Limits Between Classical and Quantum Physics: Optical Dispersion and Bohr's Atomic Model

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It is commonplace to recount the history of quantum physics on the basis of phenomena that have found no satisfactory explanation in the context of so-called classical physics. This is the case of, for example, blackbody radiation, the photoelectric effect, specific heats, and series of spectral lines. This story goes in another direction: new knowledge about quantum physics not only emerged from the need to explain new phenomena that conflicted with old theoretical structures, but also from the attempts to provide a quantum explanation of phenomena, like optical dispersion, which for a long time had found a very convincing explanation in old physical models, such as the resonance model. The boundary between classical and quantum domains of knowledge was not fixed a priori, but historically negotiated in the context of specific problems, including the problem of optical dispersion.

1. Classical Theories of Optical Dispersion

Optical dispersion consists of the scattering of light in different directions according to its color when passing through a transparent, prismatic medium. This effect is described by the dependence of the index of refraction n on the light frequency ν . Although easy to observe and to experimentally reproduce, optical dispersion has been a rather difficult phenomenon to explain, as it lies at the border between theories of light and matter.

In the early 1870s, both experimental and theoretical developments led to a radically new understanding of optical dispersion that played a paradigmatic role in optics over the ensuing 50 years.^[1] In the early 1870s, the German physicist August Kundt experimentally established that when light passed through certain media it did not spread continuously over the whole spectrum of colors. Instead, the resulting spectrum was discontinuous exactly at certain frequencies, characteristic of the prismatic medium, at which light was absorbed, instead of being dispersed.

Such a phenomenon could be well explained by using a novel model of light–matter interactions that Wolfgang Sellmeier, an almost unknown German physicist, introduced for the first time in optics in 1872. It was commonplace to regard light as consisting of propagating waves (first ether waves, then, since the

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1890s, electromagnetic waves). According to the new model, matter consisted of microscopic particles that vibrated harmonically at specific, characteristic frequencies around equilibrium positions. When the frequency of incoming light coincided with some characteristic frequency of matter particles, light and matter were set into resonance and light was absorbed. For the rest of the frequencies, light was transmitted with a phase difference, and thus dispersed. The corresponding formula describing an abrupt change in the index of refraction *n* in the neighborhood of the resonance frequencies v_i , fitted perfectly with the experimental data^[2] (Figure 1):

$$n^2 - 1 = \sum_i \frac{K_i}{\nu_i^2 - \nu^2}$$

 K_i was a parameter that represented a kind of strength of dispersion.

Such a model was a breakthrough in optics and for decades would play a paradigmatic role in the general understanding of light–matter interactions. Until the 1920s, all theories of optical dispersion made use of the same fundamental model, which was embedded over time into different conceptual and experimental frameworks.^[3] In the 1890s, the model was translated into electromagnetic language and in the early 1900s, the microscopic particles of matter were identified as electrons.

In 1904 the German physicist Paul Drude suggested that, by simply assuming that the strength of dispersion, represented by the parameter K_i , was proportional to the hypothetical number N_i of dispersion electrons resonating at v_i , it was possible to infer N_i from experiments. In this case:

$$K_i = \frac{4\pi N_i e^2}{m}$$

e and *m* were the charge and mass of the electron, respectively. Thus, the resonance model did not simply offer a description of data, but a way to analyze the microstructure of matter through optical experiments.

2. Optical Dispersion and the Boundary Between Classical and Quantum Physics

In 1913, the resonance model was for the first time at odds with a new microscopic model of matter. That year, the young Danish physicist Niels Bohr laid down the first quantum model of the





Figure 1. Plot of the dispersion formula in the neighborhood of two resonance frequencies.



Figure 2. Niels Bohr and Arnold Sommerfeld in 1919. Reproduced with permission. Copyright the Niels Bohr Archive, Copenhagen.

atom, according to which light and matter exchanged energy in a way radically different to the process of resonance that explained optical dispersion.^[4] Bohr considered atoms as microscopic planetary systems and postulated that within them electrons revolved around the nucleus in stationary orbits, from which no energy was radiated. From the point of view of ordinary electrodynamics, this was unthinkable. But still more inconceivable was that the emission and absorption of light by atoms was produced through instantaneous jumps of electrons between two different stationary orbits. Then the frequency of light ν did not coincide with the frequency of any mechanical motion of particles, as in the case of the resonance model, but was determined by the difference in energies of the two stationary states involved in the quantum jump, by means of the expression $E_1 - E_2 = hv$, h being Planck's famous constant. Therefore, Bohr's model meant a radical break with the resonance model.

Leaving aside the deep conceptual conflict between Bohr's model and the resonance model, the former had important advantages. Among them, it was very successful in describing the Balmer series of spectral lines of the hydrogen atom. The frequencies of spectral lines were supposedly caused by quantum jumps.

To be sure, Bohr's atom did not receive wide acclaim immediately. The first reactions towards Bohr's atomic model in Continental Europe expressed either rejection or skepticism. For example, Arnold Sommerfeld (**Figure 2**), director of the new Theoretical Physics Institute at the University of Munich, after having received a personal copy of Bohr's trilogy, told him: "I am still rather skeptical about atomic models in general".^[5] Nevertheless, he soon came to appreciate Bohr's atomic model, for it seemed a good candidate to explain the Zeeman and Stark effects.^[6] Actually, in 1916, Sommerfeld published a two-part paper where he brilliantly extended Bohr's model to non-circular orbits and generalized it for any degree of freedom.^[7] This paper significantly contributed to the rapid spread of Bohr's atomic model within the scientific community.

Yet Sommerfeld's famous 1916 paper was not his first contribution to Bohr's atomic model. This was in 1915 and it dealt with optical dispersion.^[8] As a matter of fact, the Dutch physicist Peter Debye, who had been Sommerfeld's first assistant in Munich, had already attempted an explanation of optical dispersion in the context of Bohr's atomic model, for the case of the hydrogen molecule.^[9] Sommerfeld generalized Debye's theory and, most importantly, took it as an opportunity to discuss, in general terms, the relationship between ordinary mechanics and electrodynamics, on the one hand, and the new quantum theory, on the other. The basic idea was that light and matter could interact in two complementary ways: on the one hand, electrons performed quantum jumps to give rise to spectral lines. On the other hand, electronic orbits could be mechanically perturbed by electromagnetic light. The second mechanism allowed light and matter to interact through resonance, the difference being that, now, the characteristic frequencies of matter at which light and matter resonated would not correspond to the frequencies of electrons vibrating around their fixed positions, but to the frequencies of electrons being harmonically perturbed from their stationary orbits. The above formula remained structurally untouched.

According to Sommerfeld, the new theory of dispersion corroborated the peaceful coexistence between what he dubbed "classical" physics (referring to electrodynamics and mechanics) and quantum physics.^[8] Sommerfeld's use of the word "classical" here is very significant. By no means the concept of "classical" was self-evident at that time in physics. It was indeed historically shaped in the context of the emerging relativity and quantum theories, when discussing specific problems like optical dispersion. The word "classical" was used to emphasize the contrast between the old and the new.^[10] Did optical dispersion belong to classical or quantum physics? According to Sommerfeld, optical dispersion remained classical, for the continuous spread of colors, only interrupted at specific frequencies, remained satisfactorily explained by a typically classical model, to wit, the resonance model. Instead, quantum physics, epitomized by quantum transitions, explained the discrete features of spectral lines. Hence the two domains of knowledge peacefully coexisted as long as they referred to two sharply differentiated phenomena. In 1917, Sommerfeld added that quantum jumps would apply to atoms, whereas resonance would take place within molecules. "Is there any contradiction in the different treatment of atom and molecule?" Sommerfeld asked himself in 1917.^[11] "Nein!" he categorically answered.

Despite Sommerfeld's enthusiasm, his theory of optical dispersion fell apart in the ensuing years, together with the divide he asserted between classical and quantum physics. The point was that Sommerfeld had ignored certain optical dispersion experiments performed in the late 1900s and early 1910s with monatomic hydrogen gas and sodium vapor, from which it was perfectly clear



Figure 3. Rudolf Ladenburg (left), Werner Heisenberg (on his left side) and Arnold Sommerfeld (in front of Ladenburg) in Göttingen, 1922. Reproduced with permission. Copyright the Niels Bohr Archive, Copenhagen.

that the characteristic frequencies at which optical dispersion was discontinuous, namely, at which light and matter should hypothetically be set into resonance, coincided in reality with the spectral lines of these substances. That is to say, if one accepted Bohr's atomic theory, whatever the mechanism causing dispersion, the characteristic frequencies v_i of the formula above should be caused by quantum jumps, instead of by a resonance process. How to retain the empirically successful dispersion formula without having recourse to resonance as the mechanism of light–matter interactions?

3. Optical Dispersion Must Be a Quantum Phenomenon

It was the German experimental physicist Rudolf Ladenburg (**Figure 3**). Who took the first steps towards a reorientation of the problem in 1921,^[12] in this case involving a redefinition of the boundary between classical and quantum physics. In Ladenburg's hands, dispersion was reinterpreted as a quantum phenomenon. Ladenburg was a theoretically skilled experimentalist at the University of Breslau and he knew very well that Sommerfeld's theory could not hold. Ladenburg had been one of the few experimentalists dealing with anomalous dispersion through monatomic gases in the years before 1913, who had found a close connection between this phenomenon and the phenomenon of spectral lines. Ladenburg's experimental program was precisely the study of dispersion around spectral lines.^[13,14]

Ladenburg's dispersion experiments prior to 1913 bore some relevant fruits. First, the dispersion formula was experimentally confirmed around the various spectral lines. Second, Ladenburg inferred from experimental results that the current interpretation of the parameter K_i in the formula was not fully satisfactory. K_i could not simply be considered proportional to the number

of optically active electrons present in the sample. Instead, the numerator of the formula should refer to some as yet unknown property of atoms and molecules in the way they interact with light.^[14]

After World War I, Ladenburg became a staunch supporter of Bohr's atomic model. With his 1921 quantum reinterpretation of dispersion, he killed two birds with one stone. First of all, Ladenburg identified the characteristic frequencies of dispersion directly with the frequencies corresponding to quantum jumps in Bohr's atom. Secondly, Ladenburg solved the interpretative problem he had encountered between 1908 and 1912 in his dispersion experiments with atomic gases. Specifically, the abovementioned unknown property of atoms and molecules in their way to interact with light was identified as their tendency to perform quantum jumps at each characteristic frequency, which was quantified through Einstein's probability coefficients, introduced in 1916.^[15] In this way the above formula remained structurally untouched, but the parameters v_i and N_i acquired a completely different physical meaning. v_i referred to the transition frequencies between two states k and j and N_i was to be re-understood in terms of the corresponding transition probabilities (a_{ki}) , the number *N* of atoms or molecules in the state *j* and the occupation of stationary states (g_k and g_i). Specifically:

$$N_i = N \frac{g_k}{g_j} a_{kj} \frac{mc^3}{8\pi^2 e^2 v_i^2}$$

Thus in Ladenburg's hands, optical dispersion became a quantum phenomenon, for it depended on quantum transitions. Yet Ladenburg had not produced any new theory of light-matter interaction. How some kind of mechanism based on quantum jumps could produce a continuous spread of colors remained unexplained. After all, optical dispersion amounted to the continuous spread of light around the characteristic frequencies, instead of at the characteristic frequencies. Ladenburg kept the resonance formalism and reinterpreted it physically. Considerable conceptual tension between classical and quantum physics was thereby introduced. On the one hand, the resonance model continued to be mathematically valid for deriving the dispersion formula. On the other hand, this model was conceptually incompatible with the model that provided the formula with physical meaning. Ladenburg's strategy was to continue analyzing experimental data in the context of classical physics, thus using the parameter N_i for the number of dispersion electrons, while reserving "quantum language" only for the physical reinterpretation at the end.^[12] How was the dilemma between mathematical model and physical interpretation solved?

4. Toward Quantum Mechanics

Ladenburg's 1921 contribution had a special impact in Copenhagen, in the context of Bohr's newly-established Institute for Theoretical Physics. Ladenburg's reinterpretation paper fitted very well with Bohr's ideas about a comprehensive account of quantum physics, epitomized in his well-known and rather elusive correspondence principle.^[16] At the core of Bohr's reasoning was the formal analogy between quantum theory and classical electrodynamics. More specifically, a classical description



Figure 4. Hendrik A. Kramers. Reproduced with permission. Copyright the Niels Bohr Archive, Copenhagen.

of systems approximated quantum results in the limit of high quantum numbers (i.e., for large orbits and large energies). For instance, the harmonic frequencies of a classical system of orbiting electrons expressed as a Fourier series coincided numerically with the quantum transition frequencies in the asymptotic limit. Bohr's idea was to find a generalized account of quantum physics by exploring more deeply these formal analogies. In 1923, Bohr mentioned Ladenburg's paper as a clear example of the close analogy between classical and quantum physics: the reaction of quantum atoms to light was formally the same as the reaction of a number of harmonic oscillators in classical theory, whose characteristic frequencies were the same as the quantum frequencies.^[17]

The first to conceive a quantum theory of optical dispersion in these terms, based on Bohr's correspondence principle, was Bohr's assistant, the Dutch physicist Hendrik A. Kramers (**Figure 4**), in 1924.^[18] Kramers's theory reflected one essential difference between classical and quantum physics: according to classical physics, at the resonance frequencies, only absorption took place. According to quantum physics, at the characteristic frequencies, light could be both absorbed and emitted, depending on whether the electrons jumped from the state of lower energy to the state of higher energy, or the other way around. Such a feature of quantum physics had a counterpart in Kramers's new dispersion formula, which amounted to a balance between absorption and emission contributions. Kramers's formula continued to bear a structural resemblance to the previous formulas, but it included a negative term. In particular, Kramers calculated the electric polarization of matter, which was proportional to $n^2 - 1$:

$$P = E \sum_{i} \frac{a_{i}^{a} \tau_{i}^{a} e^{2}}{4\pi^{2} m} \frac{1}{\nu_{i}^{2} - \nu^{2}} - E \sum_{j} \frac{a_{j}^{e} \tau_{j}^{e} e^{2}}{4\pi^{2} m} \frac{1}{\nu_{j}^{2} - \nu^{2}}$$

 v_i and v_j corresponded to the absorption and emission transition frequencies, respectively. The coefficients a_i^a and a_j^e were the transition probabilities for absorption and emission, and τ_i^a and τ_j^e were the decay times of classical oscillators having v_i and v_j as characteristic frequencies, respectively. *E* was the electric field applied. At the asymptotic limit, Kramers's and Ladenburg's formulas collapsed.

But the most important aspect of Kramers's theory for further developments in quantum mechanics was the introduction of new mathematical tools to derive the above two-term formula. In line with Bohr's correspondence principle, Kramers started with a classical analysis based on a Fourier decomposition of electronic motions into harmonic components. To model the influence of electromagnetic light, he used classical perturbation theory. Eventually, to transform the classical formal analysis of the problem into a quantum one, Kramers introduced two important mathematical rules: First of all, he replaced the classical resonance frequencies with quantum frequencies, Secondly, he substituted the differential of any function Φ , namely $\partial \Phi/\partial J$ (*J* being the action variable), with the difference $\Delta \Phi/h$ in quantum physics.^[19] This is how Kramers's dispersion formula became a difference between two terms.

In the same year 1924, Kramers's new mathematical tools were also developed by the German physicist Max Born^[20] and the American physicist John Van Vleck^[21] in their attempts to derive Kramers's two-term formula. As a matter of fact, Kramers's 1924 papers had just been very short notes, without a complete derivation of his results. Most importantly, the two substitution rules offered a unique opportunity to think more generally about the relationship between classical and quantum physics, beyond the specific case of dispersion. According to Born, a new quantum mechanics could be constructed on the basis of the substitution rules. Kramers's theory of dispersion did indeed play an important role in the path of the German physicist Werner Heisenberg towards matrix mechanics. In 1925, during Heisenberg's short stay in Copenhagen, he and Kramers together published the first full-fledged derivation of Kramers's dispersion theory.^[22] They elaborated on the substitution rules and the idea that radiative frequencies also could be the result of a sequence of various transitions.

In the same year 1925, Heisenberg published the foundational paper for matrix mechanics, the so-called "Umdeutung" paper, in which he regarded Kramers's dispersion theory as one of the "most important first steps toward such a quantumtheoretical mechanics".^[23] Heisenberg's idea was to devise a general framework to translate the classical mathematical characterization of electronic motion via Fourier series into a quantum account. Completely new rules for combining frequencies, amplitudes and phases emerged from Heisenberg's analysis, laying the groundwork for matrix mechanics.^[24] What remained of optical dispersion were the substitution rules and the idea, drawn from ref. [22], that radiative frequencies could be the result of a sequence of various transitions. Resonance had disappeared as a physical notion. In this process, the resonance model became a mathematical tool, which did not physically represent the process described. Yet thinking in terms of the resonance model as a formal analogy was productive insofar as it led to the right dispersion formula and to the development of new mathematical techniques (the two substitution rules) that, once generalized, allowed physicists to transform a genuinely classical account into a quantum one.

All in all, the persistence of the dispersion formula in experimentally describing the phenomenon turned optical dispersion into an ideal conceptual laboratory to explore new strategies to keep the resonance model as a formal structure, while relinquishing resonance as a physical mechanism. In this way the problem of optical dispersion taught physicists important lessons about how to cross the boundary between classical and quantum physics in order to gain novel insights about quantum theory. The quantum reinterpretation of optical dispersion in 1921 was a fundamental step in this direction. Yet Sommerfeld's dispersion theory was not a failure. It led to a better understanding of the limits between classical and quantum physics. Quantum and classical physics were constructed at the same time that their boundary was being defined and re-defined in the context of particular problems.

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Conflict of Interest

The author declares no conflict of interest.

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- [2] Sellmeier did not consider frictional forces. Other physicists took them into account, but Sellmeier's formula continued to be a good approximation in most cases.
- [3] By resonance model, I mean the very general notion of resonance process taking place between light and matter, and the mathematical formulation of an abrupt behavior of n at the resonance frequencies. So defined, the resonance model was closely associated to the exper-

imental pattern of dispersion with discontinuities at the characteristic frequencies of matter. Ever since the early 1870s, this model was instantiated by different dispersion theories that relied on different, specific theories of light and matter.

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